On the exact solution of the mixed-spin Ising chain with axial and rhombic zero-field splitting parameters

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Abstract

Ground-state phase diagram of the mixed spin-1/2 and spin-1 Ising chain with axial and rhombic zero-field splitting parameters is exactly calculated within the framework of the transfer-matrix method. It is shown that the rhombic zero-field splitting parameter prefers the magnetically ordered phase instead of the disordered phase.

PACS numbers: 05.50.+q; 05.70.Jk; 75.10.Pq

I. INTRODUCTION

Exactly solved one-dimensional quantum spin models traditionally belong to the most fascinating research areas as they provide valuable insight into otherwise hardly understandable aspects of cooperative and quantum phenomena [1]. In this work, we will exactly treat the mixed spin-1/2 and spin-1 Ising chain with axial and rhombic zero-field splitting parameters.

II. MODEL AND ITS EXACT SOLUTION

Consider the Ising model for a chain consisting of the alternating spin-1/2 and spin-1 atoms, which accounts also for axial and rhombic zero-field splitting parameters. The total Hamiltonian of this spin system can be written as a sum of two terms $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{ex} + \hat{\mathcal{H}}_{zfs}^{(1)}$. The former term accounts for the Ising-type exchange interaction between the nearest-neighbor spins

$$\hat{\mathcal{H}}_{ex} = -J \sum_{k=1}^{N} \hat{S}_k^z (\hat{\sigma}_k^z + \hat{\sigma}_{k+1}^z), \tag{1}$$

and the latter term accounts for the axial (D) and rhombic (E) zero-field splitting (ZFS) parameters acting on the spin-1 atoms only

$$\hat{\mathcal{H}}_{zfs}^{(1)} = -D \sum_{k=1}^{N} (\hat{S}_k^z)^2 - E \sum_{k=1}^{N} [(\hat{S}_k^x)^2 - (\hat{S}_k^y)^2]. \tag{2}$$

Above, $\hat{\sigma}_k^z$ and $\hat{S}_k^\alpha (\alpha = x, y, z)$ denote standard spatial components of the spin-1/2 and spin-1 operators, respectively, N denotes a total number of spin-1/2 (spin-1) atoms and the periodic boundary condition $\sigma_{N+1} \equiv \sigma_1$ is imposed for further convenience. It is worthwhile to remark that there is one-to-one correspondence between the Hamiltonian $\hat{\mathcal{H}}_{zfs}^{(1)}$ given by Eq. (2) and the Hamiltonian with three different parameters D^x, D^y and D^z

$$\hat{\mathcal{H}}_{zfs}^{(2)} = -D^x \sum_{k=1}^{N} (\hat{S}_k^x)^2 - D^y \sum_{k=1}^{N} (\hat{S}_k^y)^2 - D^z \sum_{k=1}^{N} (\hat{S}_k^z)^2. \tag{3}$$

The equivalence between $\hat{\mathcal{H}}_{zfs}^{(1)}$ and $\hat{\mathcal{H}}_{zfs}^{(2)}$ can easily be verified by establishing a rigorous mapping correspondence between the relevant interaction terms appearing in the Hamiltonians (2) and (3). The total angular momentum of the spin-1 atoms is integral of motion $\hat{\mathbf{S}}_k^2 = (\hat{S}_k^x)^2 + (\hat{S}_k^y)^2 + (\hat{S}_k^z)^2 = 2$ and hence, one of three parameters D^x, D^y and D^z must

depend on the other two. Consequently, the Hamiltonians $\hat{\mathcal{H}}^{(1)}_{zfs}$ and $\hat{\mathcal{H}}^{(2)}_{zfs}$ differ one from the other just by some constant factor $\hat{\mathcal{H}}^{(1)}_{zfs} = \hat{\mathcal{H}}^{(2)}_{zfs} + C$, whereas the relevant interaction terms C, D and E are connected to the ones D^x, D^y and D^z through the mapping relations

$$C = D^x + D^y,\ D = D^z - \frac{D^x + D^y}{2},\ E = \frac{D^x - D^y}{2}. \tag{4}$$

The model under investigation thus turns out to be equivalent to the one recently studied by Wu *et al.* [2] using the approach based on Jordan-Wigner transformation.

Here, the investigated model system will be exactly treated within the framework of transfer-matrix method [3]. First, it is useful to rewrite the total Hamiltonian as a sum of site Hamiltonians $\hat{\mathcal{H}} = \sum_k \hat{\mathcal{H}}_k$, whereas each site Hamiltonian $\hat{\mathcal{H}}_k$ involves all the interaction terms associated with the spin-1 atom from the kth lattice site

$$\hat{\mathcal{H}}_k = -J\hat{S}^z_k(\hat{\sigma}^z_k + \hat{\sigma}^z_{k+1}) - D(\hat{S}^z_k)^2 - E[(\hat{S}^x_k)^2 - (\hat{S}^y_k)^2]. \tag{5}$$

Due to a validity of commutation relation between different site Hamiltonians, the partition function can be partially factorized into the product

$$\mathcal{Z} = \sum_{\{\sigma_k\}} \prod_{k=1}^{N} \mathrm{Tr}_{S_k} \exp(-\beta\hat{\mathcal{H}}_k), \tag{6}$$

where $\beta = 1/(k_{\mathrm{B}}T)$, k_{B} is Boltzmann's constant, T is the absolute temperature, Tr_{S_k} means a trace over spin degrees of freedom of the kth spin-1 atom and $\sum_{\{\sigma_k\}}$ denotes a summation over all possible configurations of the spin-1/2 atoms. After tracing out spin degrees of freedom of the spin-1 atom, the relevant expression on r.h.s of Eq. (6) will depend just on its two nearest-neighbor spins σ_k and σ_{k+1}. Moreover, this expression can be subsequently used in order to define the transfer matrix

$$\begin{aligned} T(\sigma_k, \sigma_{k+1}) &= \mathrm{Tr}_{S_k} \exp(-\beta\hat{\mathcal{H}}_k) \\ &= 1 + 2\exp(\beta D)\cosh\left(\beta\sqrt{J^2(\sigma^z_k + \sigma^z_{k+1})^2 + E^2}\right). \end{aligned} \tag{7}$$

The rest of our exact calculations can be accomplished using the standard procedure developed within the transfer-matrix approach [3]. This rigorous technique allows one to express the partition function in terms of respective eigenvalues of the transfer matrix

$$\mathcal{Z} = \sum_{\{\sigma_k\}} \prod_{k=1}^{N} T(\sigma^z_k, \sigma^z_{k+1}) = \mathrm{Tr}T^N = \lambda^N_+ + \lambda^N_-. \tag{8}$$

In the thermodynamic limit $N \to \infty$, the free energy per unit cell can be expressed solely in terms of the largest eigenvalue of the transfer matrix

$$f = -k_{\mathrm{B}}T \lim_{N\to\infty} \frac{1}{N} \ln \mathcal{Z} = -k_{\mathrm{B}}T \ln(T_{11} + T_{12}), \tag{9}$$

where $T_{11} = T(\pm 1/2, \pm 1/2)$ and $T_{12} = T(\pm 1/2, \mp 1/2)$ were used to denote two different matrix elements of the transfer matrix defined through Eq. (7).

III. RESULTS AND DISCUSSION

Now, let us take a closer look at the ground-state behavior of the investigated model system. For simplicity, our subsequent analysis will be restricted only to the particular case with the ferromagnetic interaction $J > 0$, since the relevant change in sign of the parameter J causes just a rather trivial reversal of all the spin-1/2 atoms.

In the zero temperature limit, the first-order phase transition line given by the condition $D = -\sqrt{J^2 + E^2}$ separates the ferromagnetically ordered phase (OP) from the disordered phase (DP). The relevant spin order appearing in the OP and DP can be unambiguously defined through the eigenvectors

$$\begin{aligned}
|OP\rangle &= \otimes_k \left|1/2\right\rangle_k \left[\cos\left(\frac{\varphi}{2}\right)\left|+1\right\rangle_k + \sin\left(\frac{\varphi}{2}\right)\left|-1\right\rangle_k\right], \\
|DP\rangle &= \otimes_k \left|\pm 1/2\right\rangle_k \left|0\right\rangle_k ,
\end{aligned}$$

where the product runs over all lattice sites, the former (latter) ket vectors specify the state of the spin-1/2 (spin-1) atoms and the mixing angle φ is given by $\varphi = \arctan(E/J)$. In the DP, all the spin-1 atoms tend toward their 'non-magnetic' spin state $|0\rangle$ on behalf of a sufficiently strong (negative) axial ZFS parameter and hence, each spin-1/2 atom may completely independently choose any of two available spin states $|\pm 1/2\rangle$. However, the more striking spin order emerges in the OP, where the magnetic behavior of the spin-1 atoms is governed by a quantum entanglement of two magnetic spin states $|+1\rangle$ and $|-1\rangle$ and all the spin-1/2 atoms reside their "up" spin state $|1/2\rangle$. In this respect, the rhombic ZFS parameter gradually destroys a perfect ferromagnetic order between the spin-1/2 and spin-1 atoms, which appears in an absence of the rhombic term.

For better illustration, Fig. 1(a) depicts the ground-state phase diagram in the $E/J-D/J$ plane. The most surprising finding stemming from Fig. 1(a) is that the phase boundary

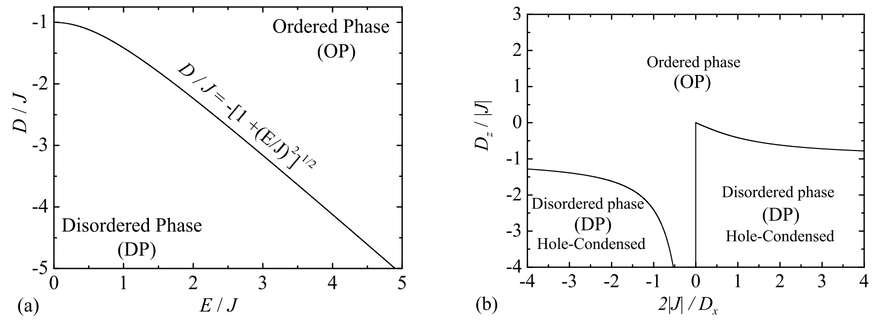

FIG. 1: Ground-state phase diagram in two different planes: (a) $E/J - D/J$ plane; (b) $2J/D_x - D_z/J$ plane for $D_y = 0$.

between OP and DP shifts toward more negative values of the axial ZFS parameter when increasing a strength of the rhombic ZFS parameter. Accordingly, it turns out that the quantum entanglement between the spin states $|+1\rangle$ and $|-1\rangle$, which is caused solely by the rhombic ZFS parameter, energetically stabilizes the OP before the DP. For comparison, Fig. 1(b) illustrates the ground-state phase diagram in the $2J/D_x - D_z/J$ plane when using Eq. (3) in order to define the ZFS Hamiltonian. Note that this phase diagram is in accord with the recent results of Wu *et al.* [2], but this phase diagram is apparently less convenient for interpreting the phase boundary between OP and DP as the parameter D_x changes according Eq. (4) both axial as well as rhombic ZFS parameters.

In conclusion, it is worthy to notice that the rigorous procedure developed on the grounds of the transfer-matrix method can readily be adapted to treat the investigated model system even in a presence of non-zero external magnetic field, which will be examined in detail in our forthcoming work.

Acknowledgments: This work was supported under the grant VEGA 1/0128/08.

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